

Statistical Physics and Computational Complexity

--- Order, Geometry and Materials

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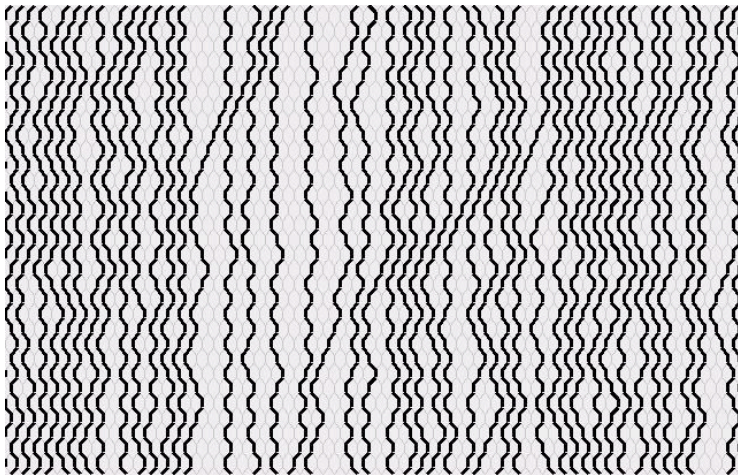
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Cris Cecka

Condensed matter & Optimization

- Common thread: complex systems with many metastable states.
- Prototypical problems.
- Deep connection between algorithms and physics: identifying relevant degrees of freedom and connections in the dynamics.
- Increased knowledge for application to other, more “standard” problems?

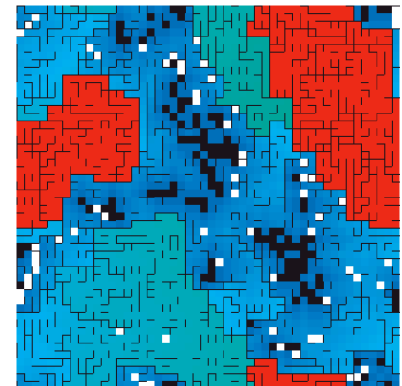
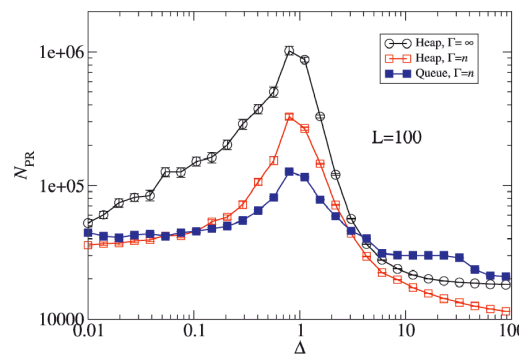
Flux lines in point AND columnar disorder.

- Response of flux lines in type-II superconductors to *transverse* fields.
- Competition between columnar disorder (straightens lines) and point disorder (causes wandering).



Random field Ising magnet.

- Empirical guide for parameters to use in algorithm.
- Explanation of algorithmic slowing down.
- Visualization of algorithm for exploration of variants.



THEORY

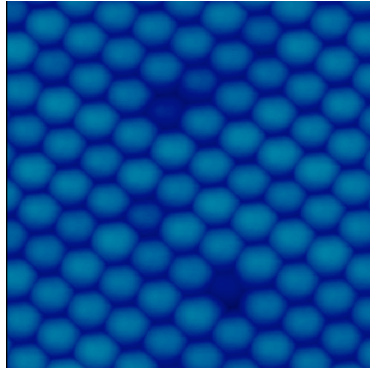
SIMULATION

EXPERIMENT

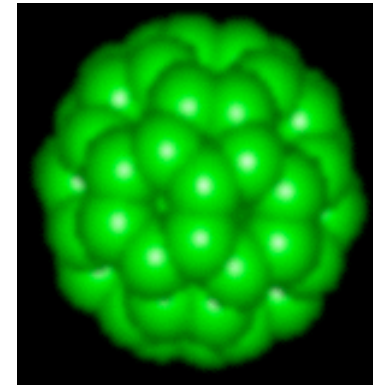
Spherical Crystals

A. Bausch et al. Science 299 (2003) 1716

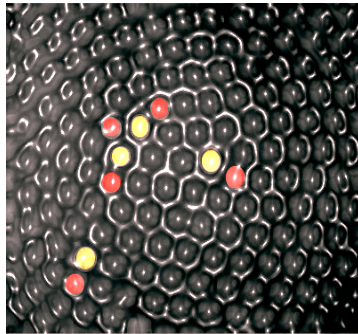
Flat space
hexagonal
close packing
of colloidal beads
with no defects –
all beads are 6-
fold coordinated.



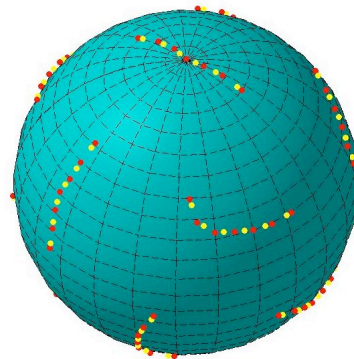
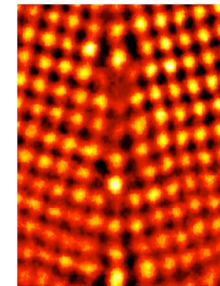
Packing on a
sphere in the
C60 buckyball.
There are 12
5-fold coordinated
vertices at the center
of the 12 pentagonal
carbon rings.

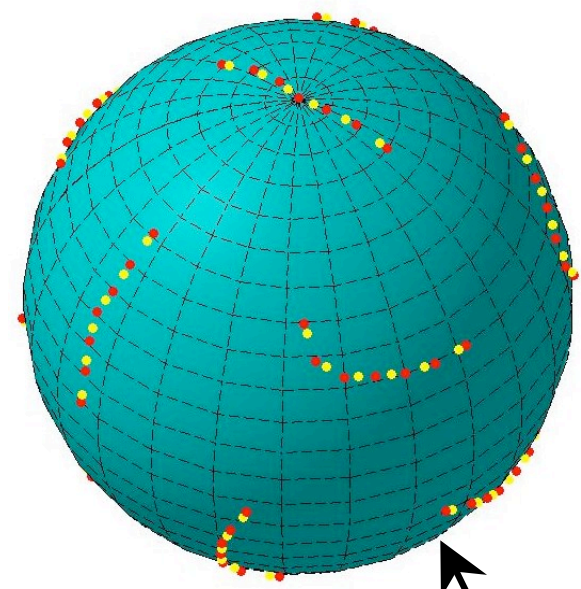
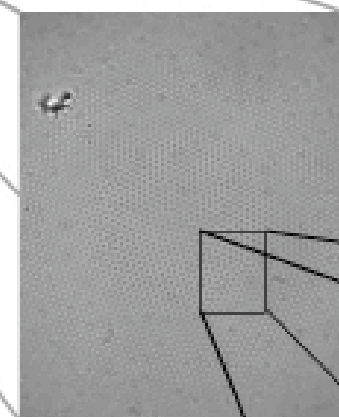
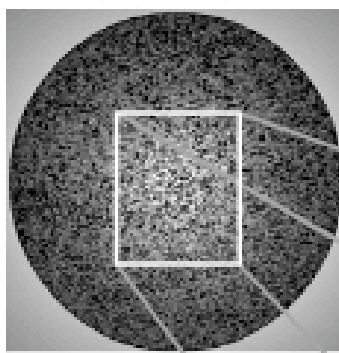


The packing of more
than 500 colloidal
beads on the
surface of a
ball leads to the
proliferation of **scars**
– these are linear
arrays of dislocations
(5-7 pairs) with one
excess disclination (5).

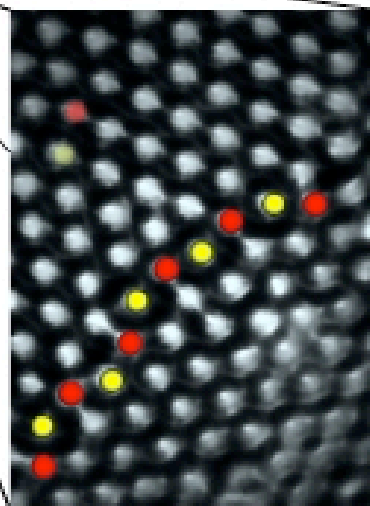


Grain boundaries in
the flat space image on
the right extend all the
way across the sample
whereas the scars to
the left (experiment)
and below (simulation)
are freely terminating.



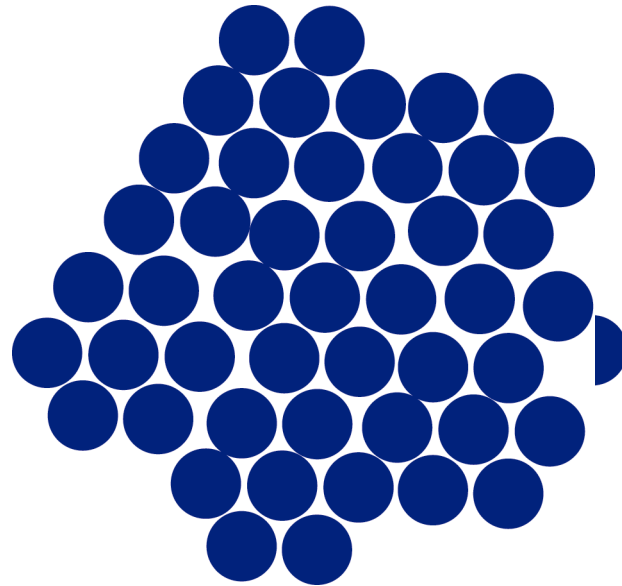


1 μm diameter beads adsorbed on spherical water droplets in oil self-assemble into 2d spherical crystals with 12 *scars* - freely terminating grain boundaries.



Theoretical defect configurations are obtained by numerical minimization of a Hamiltonian of defects in an elastic background.

Flat - Land



2 D Melting KTHNY

Liberation of:



Loss of:

1. Dislocations

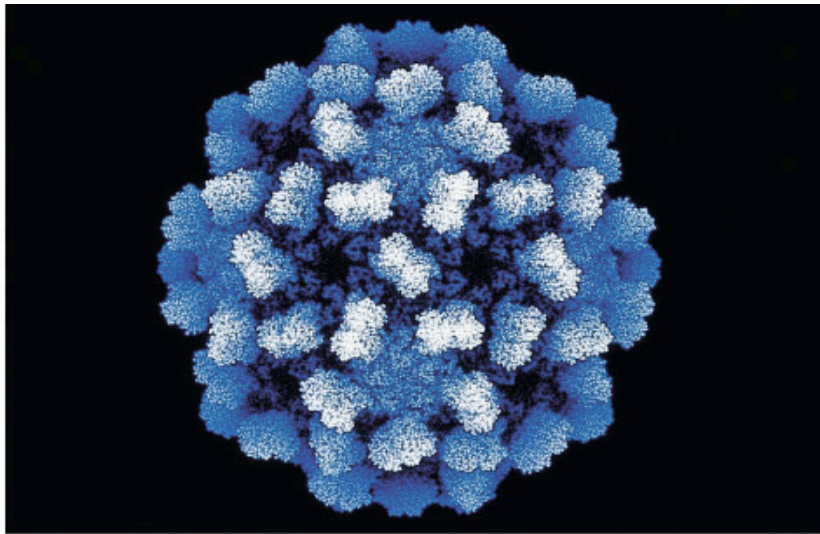
=>

Translational order

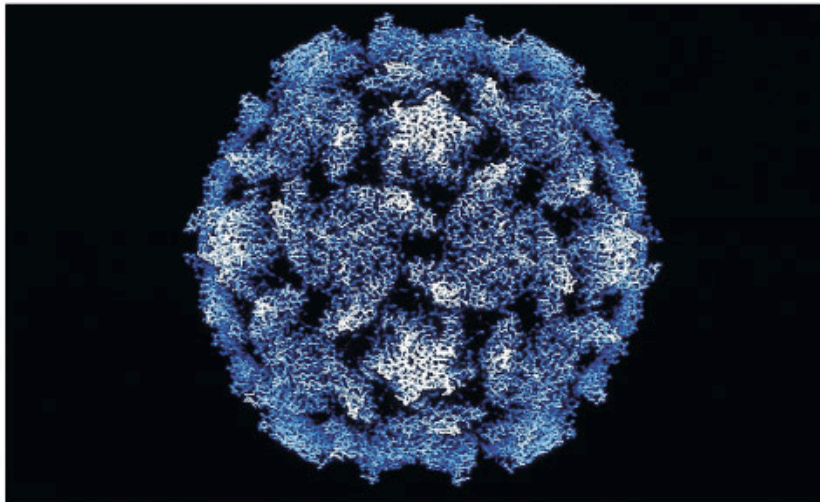
2. Disclinations

=>

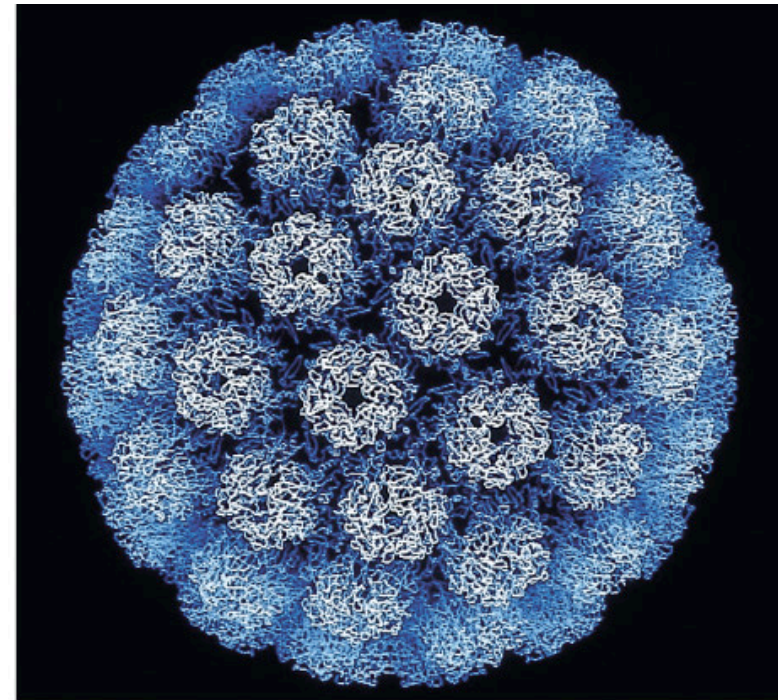
orientational order



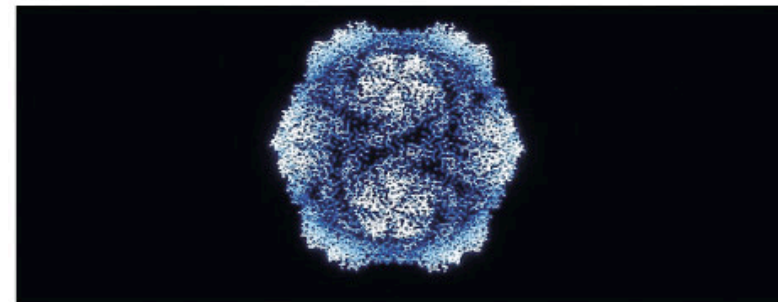
(A) Tomato bushy stunt virus



(B) Poliovirus



(C) Simian virus 40



(D) Satellite tobacco necrosis virus 20 nm

Figure 3–31 part 1 of 2. Molecular Biology of the Cell, 4th Edition.

Figure 3–31 part 2 of 2. Molecular Biology of the Cell, 4th Edition.

Cell Membranes of Erythrocytes

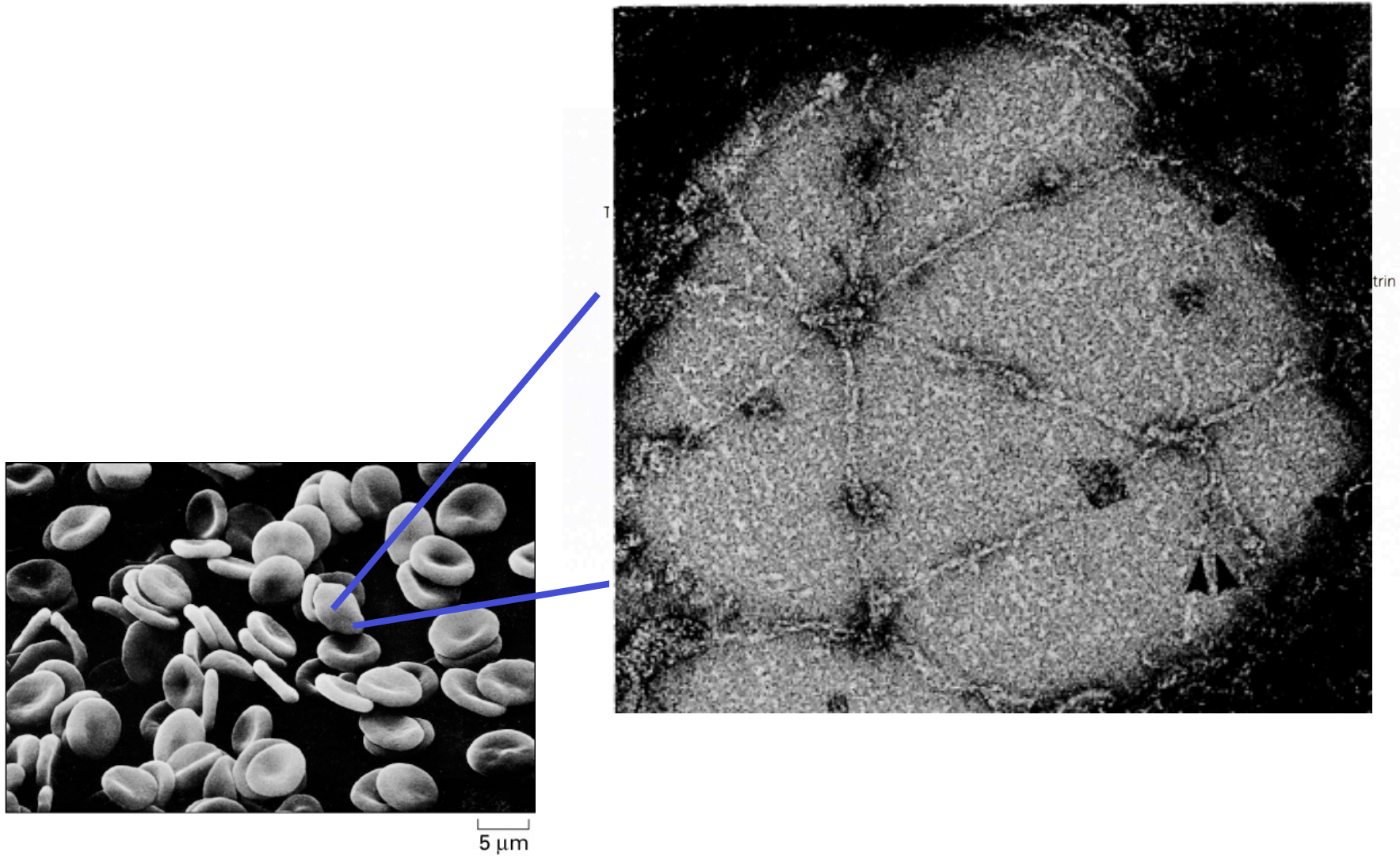
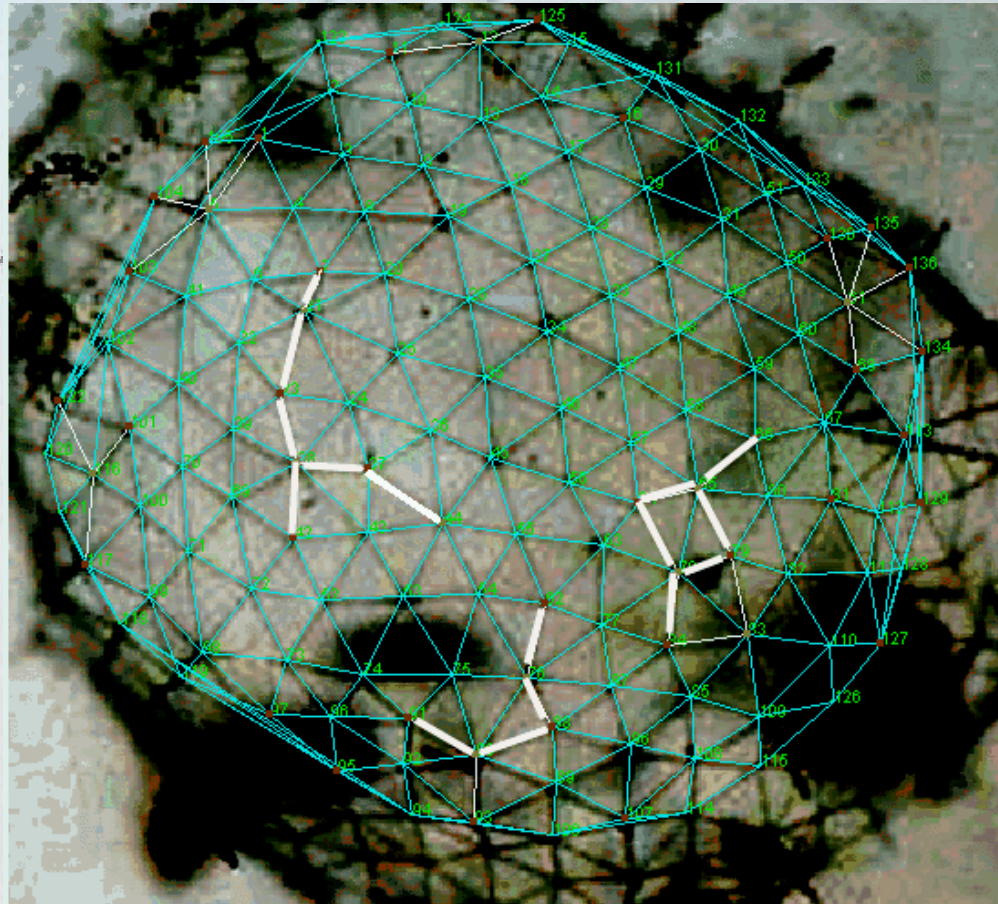
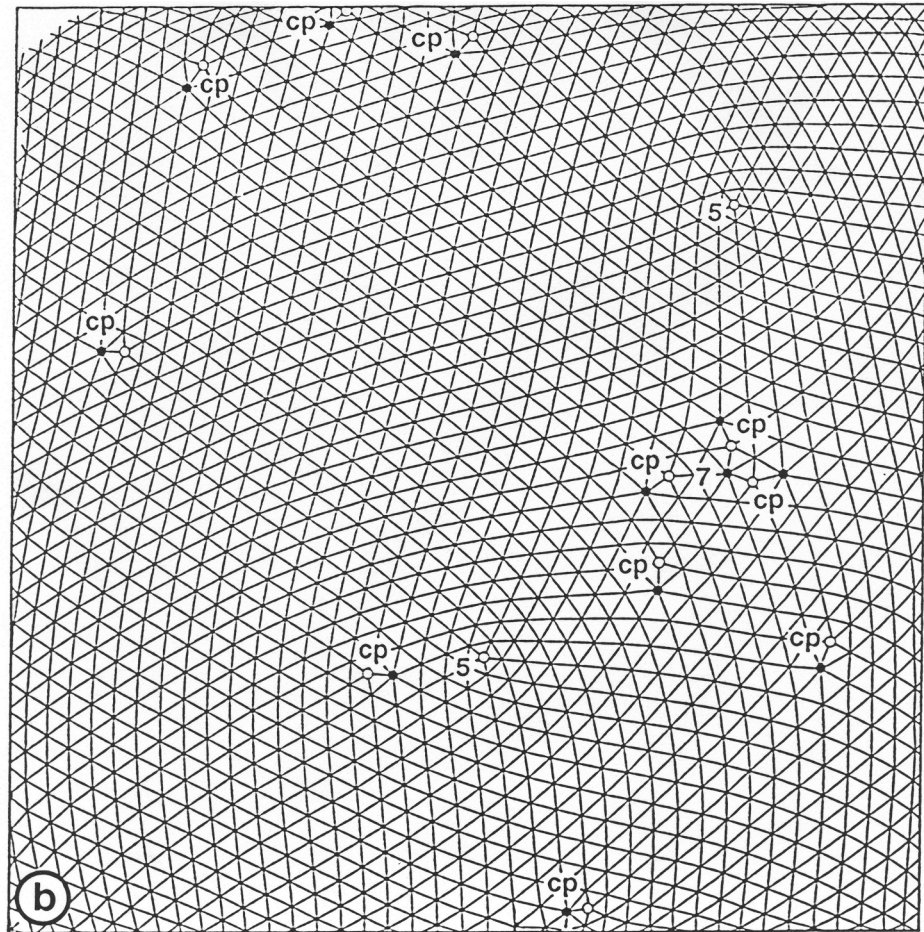


Figure 10-27. Molecular Biology of the Cell, 4th Edition.

Radiolarians



Bacterial – S-Layers



Archaeobacterium: Methanocorpusculum sinense

Pum et al., J. Bact. 173:6865- (1991)

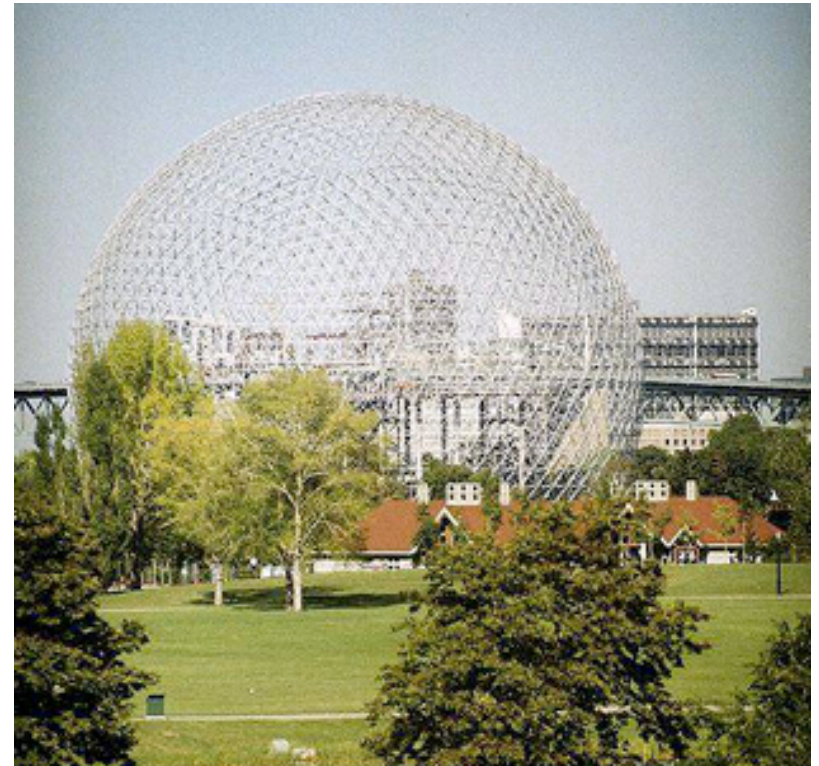
On the sphere S^2 define

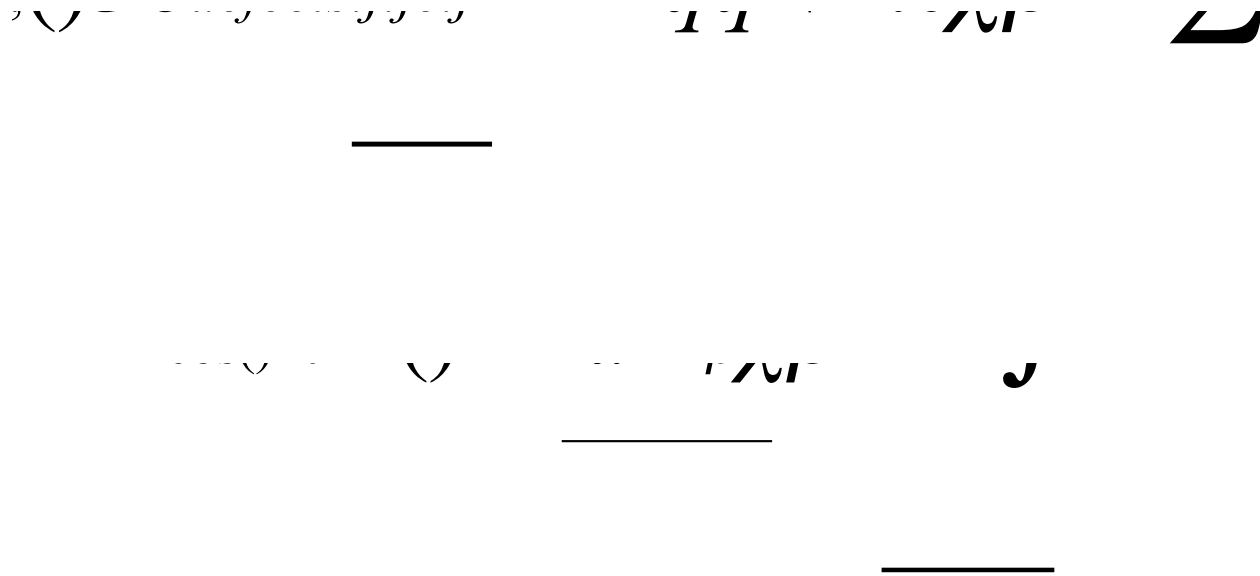
Then

The ground state for M particles on
interacting via an arbitrary pairwise repulsive
potential is the generalized Thomson problem

Map to the problem of the interacting defects
treating everything else as a continuum elastic
background

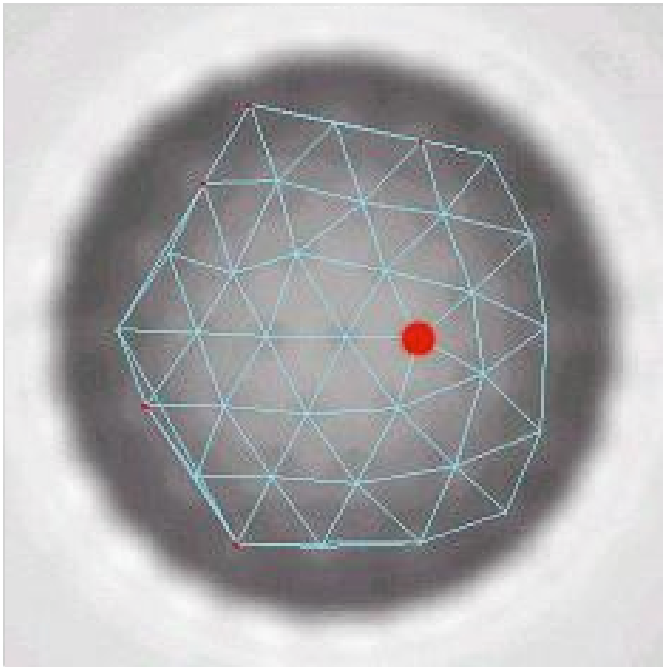
Geodesic Domes (by Buckminster)



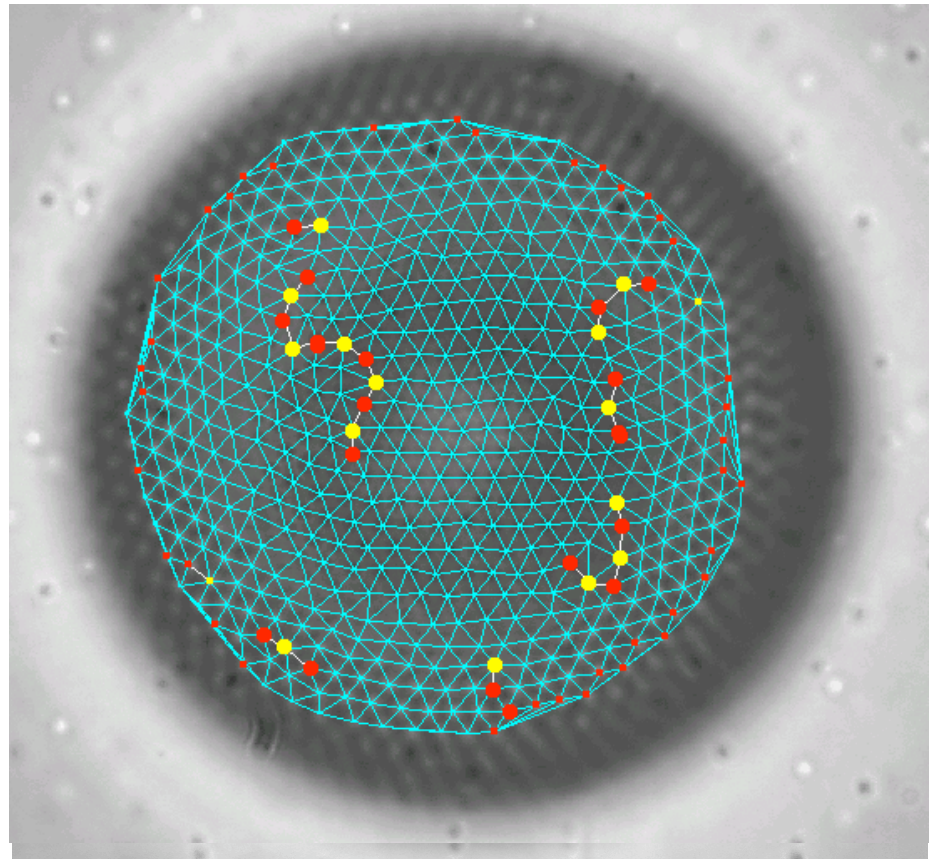


Screening of elastic strain by dislocation arrays

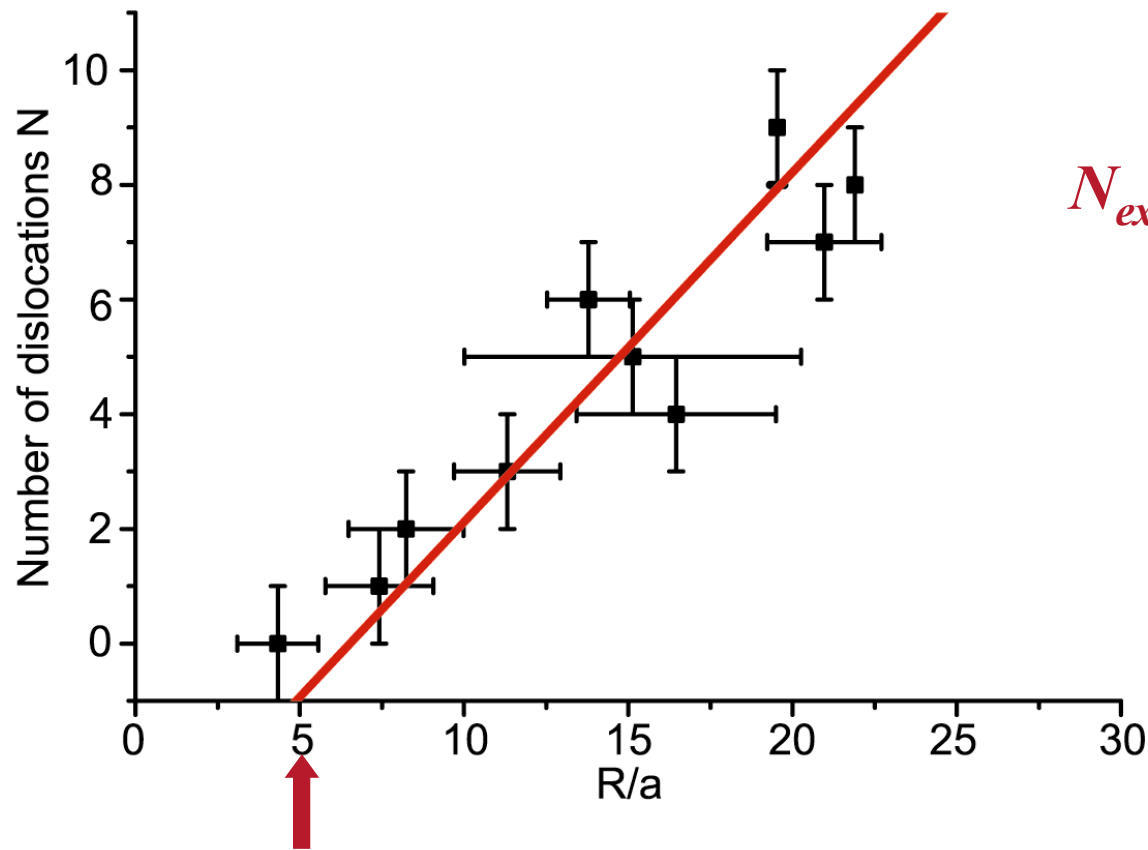
Isolated Defect



Central Defect screened by Dislocations!!!



Defect Scars



$$N_{ex} \approx 0.41 R/a$$

$$(R/a)_c \approx 5$$

Science 299:1719 (2003)

Summary

Spatial Curvature (geometry) changes order of 2d crystals

Novel grain boundaries (scars) are present at zero temperature

May lead to novel materials – supra-molecular assembly

Colloidal simulations on curved surfaces interesting